USO Polytope

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Contents

1 Introduction

A unique sink orientation is an orientation of the hypercube such that for each subcube, there exists a unique sink. It was originally proposed by Stickney and Watson [24] to study the linear complementarity problem, in which it is formulated as a digraph structure. Since then, increasing attention has been paid to it because it is highly related to other classical optimization problems. In [12], it is shown that a linear program defines a USO, and finding the unique sink in the hypercube exactly solves the programming.

Up to now, many efforts have been committed to understanding the structure of the USO itself [22] [27], proposing a fine-grained algorithm to find the global unique sink of the hypercube [11], analyze its relation to different optimization schemes [16] and other numerous aspects. Nonetheless, the relation between different USOs has not been discussed a lot, and only a little knowledge is known yet about the universal set of all possible USOs, likewise, the estimation of the number of fixed points regard to the isomorphism transformation, or what implication can be learned from finding the unique sink in a similar USO. Therefore, we try to aggregate all possible USOs together to formulate the USO polytope, of which each vertex is a single USO. In this paper, we propose several aspects to analyze the structure of the USO polytope, both locally and globally, which will better our understanding of the relationship between different USOs.

Unique Sink Orientation. Since the formal introduction of Unique sink orientation in [22], it has been found of significant importance since many specific optimization problems can be reduced to find the unique sink in USOs, including P-matrix linear complementarity problem [24] and convex quadratic programming [14]. Therefore, it is fundamental to efficiently find the unique sink of USO. However, the complexity of the problem remains an open question, the best-known algorithm for general USOs in [22] takes an exponential number of queries. [21] provides us an almost quadratic lower bound for the general case while [10] offers an expected sub-exponential upper bound for the acyclic USOs.

Apart from finding the unique sink, there also exist many open questions for understanding the structure of USO. [18] proposes an estimation for the number of USOs and [7] estimates number of the number of P-matrix USOs. Besides, in terms of the construction of USOs, [3] finds a universal construction based on the periodic tilings, and [9] proves that for each vertex of the D-cube, its L-graph is acyclic.

Although much attention is paid to specific USOs, in this paper, we consider all the general USOs as a polytope, whose vertices are the USOs. In such a way we can leverage much knowledge in combinatorial geometry and polyhedral combinatorics.

Combinatorial Geometry. This topic usually deals with combinations and arrangements of geometric objects and their discrete combinatorial properties. Since it was introduced by Hadwiger, Debrunner, and Klee [13] in 1955, it has been so far developed to an extent that is involved with topology, graph theory, combinatorial optimization, and many other aspects. Some significant results include [15] which shows a counterexample to Borsuk's conjecture [2] in certain high dimension, [20] which proves the Sylvester-Gallai Theorem [26].

Polyhedral Combinatorics. Topics in this area usually study the problems of describing the faces of the convex polytope, accessing the combinatorial property of the polytope graph, and also application of the theory of polyhedron and linear systems to combinatorics. An interesting problem among these is counting the number of the faces and [19] proves that asymptotically, there are at most $n^{\lfloor d/2 \rfloor}$ faces for d-dimensional polytope with n vertices. Another important topic in this area falls on the 0/1-polytope, which is indeed the USO polytope belongs to, and [1] proves that each Birkhoff polytope (a subclass of 0/1-polytope) can be described as two types of linear inequality or equality.

In our paper, particularly, we care more about the combinatorial meaning of the faces and symmetry group of the USO polytope.

Organization of the Paper We give some basic definitions and background knowledge about USO and polytopes in section 2, including some lemmas achieved by us. Next, we properly define the USO polytope in section 3 and introduce some necessary knowledge about the 0/1 polytope. Based on that, we try to understand the combinatorial meaning and structure of the USO polytope both locally and globally, by analyzing the faces and isometry of the polytope. Finally, we conclude this paper with several open conjectures and potential directions in the future in section 4.

Main Results

- Lemma 7 and 8, the argument about the structure of outmap and a sufficient condition for a subcube to be flippable.
- Lemma 13, Corollary 15 and Algorithm 1, theoretical and empirical analysis about the structure of USO polytope.
- Lemma 21 and 22, the argument about USO isomorphism and a sufficient condition for it to admit non-zero fixed points.
- Theorem 24 and 29, a necessary and sufficient condition for general polytope isomorphism and USO polytope automorphism.

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2 USO

2.1 Definition

The following definitions of USO are adapted from section 2 in [22], and some notations may differ.

2.1.1 Hypercube

First, we describe the structure of a hypercube.

Definition 1. *The hypercube of dimension n is an undirected graph denoted as Q_n. The vertex set is $V(Q_n) = 2^{[n]}$, and the edge set is $E(Q_n) = \{\{u,v\} | |u \oplus v| = 1\}$, where $\oplus$ denotes the symmetric set difference.*

The coordinate of vertex u is characterized by e_u, where

$$[e_u]_i = \begin{cases} 1, & i \in u, \\ 0, & i \notin u. \end{cases}$$

Another alternative notation for hypercube is in 0/1-words. A 0/1-word of length n is $u = (u_0, u_1, \cdots, u_{n-1}) \in \{0,1\}^n$. The vertex set $V(Q_n) = \{0,1\}^n$ and the edge set $E(Q_n) = \{\{u,v\} \ |d_H(u,v) = 1\}$, where $d_H(u,v) = k$ if and only if they differ in exact k positions.

Generally speaking, a subcube is an induced subgraph of a hypercube, which itself is also a hypercube.

Definition 2. *A subcube P of Q_n can be characterized by its corner u and direction A. Denote the subcube anchored at u and spanned in the set of directions $A \subseteq [n]$ as $P(u,A)$. Accordingly,*

$$V(P(u,A)) = \{u \oplus v | v \subseteq A\}.$$

For simplicity, we can assume that $u \cap A = \varnothing$, since as long as $u \setminus A = v \setminus A$, we have $P(u,A) = P(v,A)$.

Another alternative way to characterize a subcube R of Q_n is via its minimal vertex u and maximal vertex v such that $u \subseteq v$, where

$$R(u,v) = \{w | u \subseteq w \subseteq v\}.$$

Generally, the minimal subcube that covers the vertex set U is $R(\cap_{v \in U} v, \cup_{v \in U} v)$, which is called the subcube spanned by the vertex set U.

2.1.2 Unique Sink Orientation

As we formulate the hypercube as an undirected graph, an orientation of it is to assign a direction to each edge to get a directed graph Ψ_n.

Definition 3. *A unique sink orientation s of Q_n is an orientation of $E(Q_n)$ such that each subcube of Q_n has a unique sink.*

Let Ψ_n be the directed graph on $V(Q_n)$ according to s. For all $e = \{u, v\} \in E(Q_n), [(u, v) \in E(\Psi_n)] \oplus [(v, u) \in E(\Psi_n)]$.

A USO s can be characterized by its outmap function $S : 2^{[n]} \to 2^{[n]}$, where

$$S(u) = \{\lambda | (u, u \oplus \{\lambda\}) \in E(\Psi_n)\}.$$

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For each edge $e = \{u, v\}$ in the orientation s of the hypercube Q_n, the orientation indicator $I_s(u, v)$ is defined by

$$I_s(u, v) = \begin{cases} 1, & (u, v) \in E(\Psi_n), \\ 0, & (v, u) \in E(\Psi_n). \end{cases}$$

In orientation indicator words, we can alternatively define outmap $S(u)$ as

$$S(u) = \{\lambda | I_s(u, u \oplus \{\lambda\}) = 1\}.$$

Remark. In the following context, we use (u, v) to denote the undirected edge $\{u, v\}$ or the directed edge (u, v) from u to v if the orientation is specified.

2.1.3 Phase

For a specific USO s, an interesting question is how to flip some of the edges such that we get another USO s'. This problem is found to be closely related to phase. Phase is a partition of $E(Q_n)$, which is introduced in [22]. For different USOs, edges are also partitioned into phases in different ways.

Definition 4. *An edge $e = (u, v)$ is called λ-edge if $u \oplus v = \{\lambda\}$. Two different λ-edges e_1, e_2 are called in direct phase, denoted by $e_1 \| e_2$, (definition 4.7 in [22]) if there exists $u \in e_1, v \in e_2$, such that*

$$(u \oplus v) \cap (S(u) \oplus S(v)) = \{\lambda\}.$$

Specifically, for any edge e, we define $e \| e$, implying that $\|$ is reflexive and symmetric. Let $\sim$ be the transitive closure of $\|$, which is an equivalence relation. $\phi(e)$ is called the phase of edge e, and $\phi(e) = \{e' | e' \sim e\}$. A phase of a λ-edge is called λ-phase.

For more detail about the structure of USO, see section 4 in [22].

2.1.4 Polytope

The following concepts and notations about polytopes are adapted from chapter 2 in [4].

Definition 5. *Let $x_i \in X \subseteq R^n, \lambda_i \in R, i \in [k]$, then the linear combination $\sum_{i=1}^{k} \lambda_i x_i$ is called convex combination of X if*

(i) $\forall i \in [k], \lambda_i \geq 0.$

(ii) $\sum_{i=1}^{k} \lambda_i = 1.$

A linear combination $\sum_{i=1}^{k} \lambda_i x_i$ is called a conic combination if it fulfills (i) and an affine combination if it fulfills (ii).

Definition 6. *Let $X \subseteq R^n$. Then*

- *the affine hull $affn(X)$, is the set of all affine combination of X.*
- *the conic hull $cone(X)$, is the set of all conic combination of X.*
- *the convex hull $conv(X)$, is the set of of all convex combination of X.*

By definition, it is clear that $conv(X) = affn(X) \cap cone(X)$.

Hence, we can define the dimension of a point set X according to its affine hull $affn(X)$.

Definition 7. *The dimension of a point set $X \in R^{n\times m}$, denoted as $dim(X)$, is determined by its affine hull $y = affn(X)$,*

$$dim(X) = \min\{k \in \mathbf{N} : \exists A \in R^{n\times n}, rank(A) = n - k, \forall x, y \in X, Ax = Ay\}.$$

In other words, if there exists a matrix A with rank at least $n-k$, and $\forall x, y \in X$, we have $x - y \in ker(A)$, it is implied that X has dimension as most k.

Definition 8. *Let $w \in R^n \setminus \{0\}$ and $b \in R^n$. Then the $n-1$ dimensional subspace $H_{w,b} = \{w^\top x + b = 0\}$ is called a hyperplane of R^n.*

Accordingly, a hyperplane $H_{w,b}$ defines a positive half-space H^+ and a negative half-space H^- respectively:

- $H^+ = \{x \in R^n | w^\top x + b \geq 0\}$

- $H^- = \{x \in R^n | w^\top x + b \leq 0\}$

Definition 9. *Let $A \in R^{m\times n}$ and $b \in R^m$, the set $P = \{x \in R^n | Ax \leq b\}$ is called a polyhedron, and a bounded polyhedron is called a polytope.*

As it is defined, a polytope can be regarded as the intersection of finite many half-spaces. Meanwhile, it is also a convex hull of finitely many vertices.
REMARK. Without specification, in the following sections, we always talk about nonempty and bounded polyhedrons.

Definition 10. *Let P be a polyhedron, a hyperplane H is called as a supporting hyperplane of P if $P \cap H \neq \varnothing$, and either $P \subseteq H^+$ or $P \subseteq H^-$.*

Specifically, for a supporting hyperplane H and $x, y \in P$, if $x \in P \cap H$ and $y \notin P \cap H$, we say that H supports P on x and excludes y respectively.

Definition 11. *Let $P \subseteq R^n$ be a polyhedron and $dim(P) > 0$, a d-dimensional face f with $dim(f) = d$ is either P itself, the empty set or the intersection of P and some supporting hyperplane H. Hence, f is called*

- *a vertex, if f is a 0-dimensional face.*
- *an edge, if f is a 1-dimensional face.*
- *a facet, if f is a $(dim(P) - 1)$-dimensional face.*

Besides, an empty set $\varnothing$ is usually regarded as a (-1)-face.

By definition, to validate either f is a face of P, it is equivalent to validating whether there exists a supporting hyperplane H such that H supports P on f and excludes any other points. However, this is not feasible as we may have uncountable infinite points in P.

Therefore, we conclude the definitions of polytope by the following lemma.

Lemma 1. *Let $X \subseteq R^n$ be a set of points in R^n, $P = conv(X)$. Let $X' \subseteq X, S = X \cap conv(X'), T = X \backslash S$ and $S \neq \varnothing, T \neq \varnothing$. Then $conv(S)$ is a face of P if and only if there exist a hyperplane $H_{w,b} : \{x | f(x) = w^\top x + b = 0\}$, such that $\forall x \in S, f(x) = 0$ and $\forall x \in T, f(x) > 0$.*

PROOF. "$\Rightarrow$": Suppose that $conv(S)$ is a face of P, then there exists H such that $P \cap H = conv(S)$ and $P \subseteq H^+$, and hence $T \subseteq H^+$. Notice that $T \cap conv(S) = \varnothing$, thus $T \cap H = \varnothing$. Therefore, $\forall x \in S, x \in conv(S) \subseteq H$, $f(x) = 0$. Hence, $\forall x \in T$, $x \notin H$, $x \in H^+ \setminus H$, and $f(x) > 0$.

"$\Leftarrow$": Suppose that there exist such hyperplane H, and we will prove that $H \cap P = conv(S)$ and $P \subseteq H^+$, indicating that $conv(S)$ is a face of P.

First we argue that $P \subseteq H^+$. $\forall y \in P$, it is a convex combination of X, and $y = \sum_i \lambda_i x_i$. Therefore,

$$\begin{aligned} f(y) &= w^\top y + b \\ &= w^\top (\sum_i \lambda_i x_i) + b \\ &\overset{(a)}{=} w^\top (\sum_i \lambda_i x_i) + (\sum_i \lambda_i b) \\ &= \sum_i \lambda_i f(x_i) \overset{(b)}{\geq} 0, \end{aligned}$$

where (a) stands for $\sum_i \lambda_i = 1$, and (b) holds because $\forall i, f(x_i) \geq 0$ and $\lambda_i \geq 0$, implying that $P \subseteq H^+$.

Next, we argue that $H \cap P = conv(S)$. $\forall y \in conv(S)$, analogous to the above equation, we have $f(y) = 0$ and $y \in H$. $\forall x \in P \setminus conv(S)$, $y = \sum_i \lambda_i x_i$. Notice that $y \notin conv(S)$, there exist k such that $x_k \in T$ and $\lambda_k > 0$. Therefore,

$$f(y) \geq \lambda_k f(x_k) > 0,$$

implying that $(P \setminus conv(S)) \cap H = 0$, and $H \cap P = conv(S)$. Combined with $P \subseteq H^+$, we conclude that $conv(S)$ is a face of P. $\square$

This lemma shows that, in order to check whether f is a "nontrivial" face of the polytope P, it is equivalent to validate whether there exists a hyperplane H such that $V(f) \subseteq H$ and $V(P) \subseteq H^+$, where $V(f)$ and $V(P)$ are extreme points of the polytope f and P.

Remark. The polytope P itself and the null-face $\varnothing$ are also regarded as faces of P, which are not the intersection of P and supporting hyperplane H, and also do not belong to the cases that Lemma 1 can apply.

2.2 Structure of USO

For the hypercube Q_n, there are in total $2^{n2^{n-1}}$ ways to orient the edges. Of course, most of them are not USO, according to the upper bound of number of USOs in [18]. USOs are quite well-structured as we require each subcube to have a unique sink. However, what statement can we make about the structure of the USOs? We will try to illustrate that in this section.

Lemma 2. *Let S be the outmap of the USO s of Q_n. Let $A \subseteq [n]$, $[S \oplus A](u) := S(u) \oplus A$. $S \oplus A$ is an outmap of the orientation which flips the edges in the directions of A and it is also a USO outmap.*

PROOF. See Lemma 4.1 in [22].

Lemma 3. *Let S_Q be the outmap of the USO s of Q_n. For any subcube $P(u, A)$ of Q_n, the outmap restricted on it is $S_P(v) = S_Q(v) \cap A$, which is bijective.*

PROOF. See Lemma 4.1 in [22].

Corollary 4. *S is a outmap of a USO of hypercube Q_n, then S is a bijection from $2^{[n]}$ to $2^{[n]}$.*

PROOF. See Corollary 4.2 in [22].

Lemma 3 shows that the outmap is bijective on any subcube. Combined with corollary 4, it implies that a unique sink orientation is also a unique source orientation. In other words, each subcube has a unique source whose incident edges are all directed outgoing.

Lemma 5. *S is an outmap of a USO if and only if for any different u and v, $(S(u) \oplus S(v)) \cap (u \oplus v) \neq \varnothing$.*

PROOF. See Proposition 4.3 in [22].

Lemma 6. *For any set of directions A and USO outmap S_Q, the A-sink-inherit outmap (see section 3 in [27]) $S_{Q/A}(u), u \cap A = \varnothing$ is defined by $S_{Q/A}(u) = S_Q(v) \setminus A$, where v is the unique sink in the subcube $P(u, A)$. Hence, $S_{Q/A}$ is another USO outmap with $|A|$ dimensions lower.*

Similarly, the A-source-inherit outmap $S_{Q/A}(u), u \cap A = \varnothing$ is defined by $S_{Q/A}(u) = S_Q(v) \setminus A$, where v is the unique source in the subcube $P(u, A)$.

PROOF. See Lemma 3.1 in [27]. Here we provide an alternative proof that fits in our context.

Since $S_{Q/A/B} = S_{Q/(A \cup B)}$, we can suppose that $|A| = 1$. First, we will show that $S_{Q/A}$ is a valid outmap. In other words, $S(u)$ agrees with each other and each edge exists exactly once in the outmap of two endpoints, implying that

$$(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = d, \forall (u, v) \in Q_n/A,$$

where $d = u \oplus v$.

Consider the edge (u, v) in the subcube Q/A, we write $I_Q(u, v) = I_s(u, v)$ and $I_{Q/A}(u, v) = I_{s'}(u, v)$, where s' is the USO corresponds to the inherit outmap $S_{Q/A}$. There are two different cases.

- $I_Q(u, u \oplus A) = I_Q(v, v \oplus A)$. Suppose that $I_Q(u, u \oplus A) = I_Q(v, v \oplus A) = 0$, thus $S_{Q/A}(u) = S_Q(u), S_{Q/A}(v) = S_Q(v)$. Therefore, $(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = (S_Q(u) \cap d) \oplus (S_Q(v) \cap d) = d$.
- $I_Q(u, u \oplus A) \neq I_Q(v, v \oplus A)$. Suppose that $I_Q(u, u \oplus A) = 0$ and $I_Q(v, v \oplus A) = 1$. Notice that $(u, v, u \oplus A, v \oplus A)$ is a USO, implying $I_Q(u, v) = I_Q(u \oplus A, v \oplus A)$. Accordingly, $d \subseteq S_Q(u) \oplus S_Q(v \oplus A)$. Therefore, $(S_{Q/A}(u) \cap d) \oplus (S_{Q/A}(v) \cap d) = (S_Q(u) \cap d) \oplus (S_Q(v \oplus A) \cap d) = d$.

Next, we will show that $S_{Q/A}$ is a USO outmap. It suffices to prove that there is a unique sink in $S_{Q/A}$. Suppose that $S_{Q/A}(u) = \varnothing$, thus $S_Q(v) \subseteq A$. Since v is the unique sink in $P(u, A)$, we have $S_Q(v) \cap A = \varnothing$. Accordingly, $S_Q(v) = \varnothing$, v is also the unique sink of Q and $S_{Q/A}$ is a USO outmap. □

This lemma shows what a USO outmap S is composed of. Instead of naturally dividing Q_n into subcubes $P(\varnothing, [n-1])$ and $P(\{n\}, [n-1])$, we can also take $A = \{n\}$ and compress S into a sink-inherit outmap and a source-inherit outmap with regard to the direction A.

Lemma 2 tells us that flipping edges in certain directions of a USO can provide us with another USO, but that is quite a few. For a USO s of Q_n, there are 2^n such specific flips but we have $n2^{n-1}$ flips in total. Are there any other flips that can also lead to another USO, such as flipping an edge or flipping all the edges in a subcube? The following lemmas achieved by us will try to depict it.

Specifically, we claim without proof that, for any outmap S of a USO s, and its edge $e = (u, v)$, flipping the edge e will transform s into another USO s' if and only if $u \oplus S(u) = v \oplus S(v)$. Therefore, the function map $f_S(u) = u \oplus S(u)$ may encode the information of flippable edges.

Lemma 7. *Let s be a USO of Q_n and S be its outmap. Define $f_S(u) = u \oplus S(u)$ and $f_S^{-1}(x) = \{u | f_S(u) = x\}$. For any $x \in Q_n$, we claim $|f_S^{-1}(x)|$ is even.*

Proof. We prove this by induction. This statement holds for Q_1 clearly. Suppose that for Q_{n-1} this claim holds. Take $A = \{n\}$ and consider the outmaps restricted on the subcubes $P(\varnothing, [n-1])$, $P(\{n\}, [n-1])$ and the A-sink-inherit outmap. We introduce two auxiliary functions,

$$g_S^{-1}(x) = \{u | f_S(u) = x \wedge n \notin u\},$$
$$h_S^{-1}(x) = \{u | f_S(u) = x \wedge n \in u\},$$

and it is clear that $|f_S^{-1}(x)| = |g_S^{-1}(x)| + |h_S^{-1}(x)|$. Actually, g_S^{-1} and h_S^{-1} is a partition of the f_S^{-1} based on where the preimage u comes from.

Consider two disjoint subcubes $P_1 = P(\varnothing, [n-1])$ and $P_2 = P(\{n\}, [n-1])$. Denote the restricted outmap as $S_1(u)$ and $S_2(u)$ respectively. Therefore,

$$S_1(u) = S(u) \cap [n-1], f_{S_1}(u) = u \oplus S_1(u),$$
$$S_2(u) = S(u) \cap [n-1], f_{S_2}(u) = u \oplus S_2(u).$$

According to the induction, $|f_{S_1}^{-1}(x)|$ and $|f_{S_2}^{-1}(x)|$ are both even. Notice that $\forall u \in P_1$, either $S(u) = S_1(u)$ or $S(u) = S_1(u) \cup \{n\}$. Therefore, $f_{S_1}(u) = f_S(u)$ or $f_{S_1}(u) = f_S(u) \cup \{n\}$, indicating that $\forall x \subseteq [n-1]$,

$$|g_S^{-1}(x)| + |g_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{1}$$

Analogous to (1), we have $f_{S_1}(u) = f_S(u)$ or $f_{S_1}(u) \cup \{n\} = f_S(u)$, and then

$$|h_S^{-1}(x)| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{2}$$

Let $A = \{n\}$ and consider the A-sink-inherit outmap $S_3 = S_{Q/A}$. Since $S_3(u) = S_Q(v) \setminus \{n\}$ and v is the unique sink in $P(u, \{n\})$, $n \notin S_Q(v)$, we have $S_3(u) = S(v), f_{S_3}(u) = f_S(v) \oplus (u \oplus v)$. According to the induction, we have $|f_{S_3}^{-1}(x)|$ is even. Notice that $u \oplus v \in \{\varnothing, \{n\}\}$, thus, $\forall x \subseteq [n-1]$,

$$|g_S^{-1}(x)| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{3}$$

(1) + (3):

$$|g_S^{-1}(x \cup \{n\})| + |h_S^{-1}(x \cup \{n\})| \equiv 0 \pmod 2. \tag{4}$$

(2) + (3):

$$|g_S^{-1}(x)| + |h_S^{-1}(x)| \equiv 0 \pmod 2. \tag{5}$$

Therefore, $\forall x \in Q_n$, we have

$$|f_S^{-1}(x)| = |g_S^{-1}(x)| + |h_S^{-1}(x)| \equiv 0 \pmod 2,$$

implying that the statement also holds for Q_n, thus completing the induction. □

Lemma 8. *Let s be a USO of Q_n and S be its outmap. Suppose that there exists a subcube $P(w, A) \subseteq Q_n$ such that for any vertex $u, v \in P(w, A)$, we have $u \oplus S(u) = v \oplus S(v)$. Then, the orientation s' obtained by flipping each edge in $P(w, A)$ from s is another USO.*

Proof. To see this, first we need to argue that s restricted on $P(w, A)$ is a uniform USO. A uniform USO is an orientation such that for any λ, each λ-edge shares the same orientation.

The outmap restricted on the subcube $P(w, A)$ is $S_P(u) = S_Q(u) \cap A$. For any edge $e = (u, v)$, the orientation indicator is

$$I_s(u, v) = |S(u) \cap (u \oplus v)|.$$

Therefore, for any two λ-edge $e_1 = (u_1, v_1), e_2 = (u_2, v_2), u_1 \subseteq v_1, u_2 \subseteq v_2$, we have

$$I_s(u_1, v_1) = |S(u_1) \cap \{\lambda\}|,$$
$$I_s(u_2, v_2) = |S(u_2) \cap \{\lambda\}|.$$

Notice that $S(u_1) \oplus u_1 = S(u_2) \oplus u_2$ and $u_1 \cap \{\lambda\} = u_2 \cap \{\lambda\} = \varnothing$, we have $S(u_1) \cap \{\lambda\} = S(u_2) \cap \{\lambda\}$, indicating that $I_s(u_1, v_1) = I_s(u_2, v_2)$. Actually, for any uniform USO s, its outmap S can be characterized by its unique sink t such that $\forall u, S(u) = u \oplus t \oplus S(t)$.

Next, we need to argue that any subcube $P(u, B)$ in the orientation s' has a unique sink. Let S' be the outmap of orientation s'. There are following several cases to consider.

- $P(u, B) \cap P(w, A) = \varnothing$. Accordingly, the orientation of $P(u, B)$ in s' remains the same as in s, indicating that the sink is unique.
- $P(u, B) \cap P(w, A) = C \neq \varnothing$. For any $v \in C$, notice that $S'(v) = S(v) \oplus A$ and $S(v) = S(t) \oplus (v \oplus t)$, where t is the unique sink in $P(w, A)$. Thus, $S'(v) = S(t) \oplus t \oplus v \oplus A$. Notice that $t \oplus v \subseteq A$, then $t \oplus v \oplus A \subseteq A$. Consider the unique sink of the subcube $P(u, B)$ in the orientation s'. We can distinguish the following two cases:
  - $B \cap (S(t) \setminus A) \neq \varnothing$. Then for each vertex $v \in C$, we have $S(v) \cap B \neq \varnothing$ and $S'(v) \cap B \neq \varnothing$, indicating that each vertex in C is neither a sink of $P(u, B)$ in s nor s'. Then, the original unique sink in $P(u, B)$ remains the same.
  - $B \cap (S(t) \setminus A) = \varnothing$. Then for each vertex $v \in C$, we have $(S(v) \setminus A) \cap B = \varnothing$ and $(S'(v) \setminus A) \cap B = \varnothing$, indicating that each vertex in C has no edge directed out of C in $P(u, B)$. Therefore, the unique sink of C is exactly the unique sink of $P(u, B)$.

In all the cases discussed above, each subcube $P(u, B)$ has a unique sink, indicating that s' is another USO. $\square$

Remark. One may conjecture that for any USO s, the such edge always exists. As it is shown in Lemma 7, $\forall u \in Q_n$, there exist v other than u such that $u \oplus S(u) = v \oplus S(v)$. However, it is not the case that there always exists such adjacent u and v, and [17] implicitly shows a counter-example in dimension eight with a tiling of unit cubes. Generally, whether we can flip some edges in a USO to get another USO is closely related to phases, which will be illustrated in detail next.

Fact 9. *Let s be a USO and λ-edges e_1 and e_2 are in direct phase. Another orientation s' is obtained by only flipping e_1 in s and s' is not a USO.*

Proof. See definition 4.7 in [22].

This fact implies that to flip some specific λ-edge e to get another USO, it is necessary to flip all the edges in the phase of e or some edges adjacent to the edge e.

Lemma 10. *Let s be a USO and let L be a set of non-adjacent edges in s, essentially a matching. Flipping all the edges in L transforms s into the orientation s', and s' is also a USO if and only if L is a union of phase(s).*

Proof. See Proposition 4.9 in [22].

Remark. Notice that lemma 10 is not a generalization of lemma 8 as here we require the flipped edges to be a matching of Q_n.

3 USO Polytope

3.1 Definition

To define the USO polytope, we need to map the USOs into the euclidean space by the orientation indicator. Let $E(Q_n) = (\{u_1, v_1\}, \{u_2, v_2\}, \cdots, \{u_m, v_m)\})$ be an ordered sequence of the edges and $m = n2^{n-1}$. Let us fix an arrangement of the edges such that for any λ_1-edge $e_1 = (u_1, v_1)$ and λ_2-edge $e_2 = (u_2, v_2)$, e_1 appears before e_2 in $E(Q_n)$ if either of the following happens:

- $\lambda_1 < \lambda_2$,
- $\lambda_1 = \lambda_2 \wedge O(u_1) < O(u_2)$,

where $O(u) : 2^{[n]} \to \mathbb{N}$ implies a total order on $2^{[n]}$ and $O(u) = \sum_{i=1}^{n} 2^i [i \in u]$.

USO s of Q_n can be represented by its USO vector $p_s \in \{0,1\}^{n2^{n-1}}$. For the i-th edge $e_i = (u_i, v_i)$ in $E(Q_n)$, we take

$$(p_s)_i = I_s(u_i, v_i), u_i \subseteq v_i.$$

Definition 12. *The USO polytope P_n is defined as the convex hull of p_s, $P_n = conv(p_s)$, where s is all the possible USO of Q_n.*

The USO polytope P_n is a special case of 0/1-polytope, of which some facts we will discuss next.

3.2 0/1 Polytope

Definition 13. *A d-dimensional 0/1 polytope P is the convex hull of d-dimensional 0/1 vector set X. In other words, $\forall x \in X, x = (x_1, x_2, \cdots, x_d)$, $x_i \in \{0,1\}$ and $P = conv(X)$.*

Alternatively, we can describe each $x \in \{0,1\}^d$ with set words by the explicit mapping $f : \{0,1\}^d \to 2^{[d]}$, such that

$$f(x) = \{i | x_i = 1\}.$$

It is clear that f is bijective and its inverse f^{-1} is unique:

$$f^{-1}(y) = ([1 \in y], [2 \in y], \cdots, [d \in y]).$$

Analogous to the set operation, we can define the union and intersection operation for u and v in $\{0,1\}^d$:

$$u \cup v = f^{-1}(f(u) \cup f(v)),$$
$$u \cap v = f^{-1}(f(u) \cap f(v)),$$
$$u \oplus v = f^{-1}(f(u) \oplus f(v)).$$

For the corner $u \in \{0,1\}^d$ and direction $A \in \{0,1\}^d$ with $u + A \in \{0,1\}^d$, we define the subcube anchored at u as $P(u, A)$,

$$P(u, A) = \{u + v | f(v) \subseteq f(A)\}$$

For u and v with $f(u) \subseteq f(v)$, the minimum subcube covering u and v is defined as $R(u, v)$,

$$R(u, v) = \{w | f(u) \subseteq f(w) \subseteq f(v)\}.$$

For any set X, the minimum subcube that covers the convex hull of X is $R(\cap_{x \in X} x, \cup_{x \in X} x)$.

For simplicity, we define $u \subseteq v$ if and only if $f(u) \subseteq f(v)$. Similarly, we omit f and f^{-1} and use the set words and 0/1-vector words interchangeably in the following sections when the case is clear.

3.2.1 Vertex of 0/1 Polytope

Fact 11. *Let $P = conv(X)$ and $X \subseteq \{0,1\}^d$. Then, $\forall x \in X$, x is an extreme point (0-face) of P.*

Proof. For $x \in X$, consider the hyperplane $h(y) = (\mathbf{1} - 2x)^\top y + x^\top x = 0$. Notice that

$$\begin{aligned} h(y) &= \sum_i (y_i - 2y_i x_i + x_i^2) \\ &\overset{(a)}{=} \sum_i (y_i - x_i)^2 \geq 0, \end{aligned}$$

where (a) stands because $y_i \in \{0,1\}$ and $y_i = y_i^2$. Therefore, $h(y) = 0$ if and only if $y = x$ and the hyperplane $h(y) = 0$ only support the vertex x and excludes other points, implying that x is an extreme point. $\square$

3.2.2 Edge of 0/1 Polytope

Fact 12. *Let $P = conv(X)$ and $X \subseteq \{0,1\}^d$. For $x, y \in X$, suppose that for the subcube $R(x \cap y, x \cup y)$, $X \cap R(x \cap y, x \cup y) = \{x, y\}$, then the segment $e = (x, y)$ is an edge (1-face) of P.*

Proof. To see this, take $u = x \cap y, v = x \cup y$. Consider the hyperplane $h(z) = (\mathbf{1} - u - v)^\top z + u^\top u = 0$. Notice that

$$\begin{aligned} h(z) &= \sum_i (z_i^2 - z_i u_i - z_i v_i + u_i^2) \\ &= \sum_i (z_i(z_i - v_i) + u_i(u_i - z_i)). \end{aligned}$$

Since $u_i \leq v_i$, there are two cases to consider.

- $u_i = v_i$, then $z_i(z_i - v_i) + u_i(u_i - z_i) \overset{(a)}{=} (z_i - u_i)^2 \geq 0$,
- $u_i = 0, v_i = 1$, then $z_i(z_i - v_i) + u_i(u_i - z_i) \overset{(b)}{=} z_i(z_i - 1) = 0$,

where (a) and (b) hold since $z_i \in \{0, 1\}$.

Therefore, $h(z) = 0$ if and only if $u \subseteq z \subseteq v$, indicating that $z \in R(u, v)$. Notice that x and y are the only two vertices inside $R(u, v)$. The hyperplane $h(z) = 0$ only supports vertices x, y and excludes other vertices, thus making $e = (x, y)$ a 1-face of P. □

This fact shows that for any segment (u, v), only the vertices inside the subcube $R(u \cap v, u \cup v)$ can prevent it from becoming an edge of the polytope. Hence, the such argument can be enhanced into the following lemma.

Lemma 13. *Let $X \subseteq \{0, 1\}^d$. For any segment $e = (x, y), x, y \in X$ and the subcube $R(u, v)$ spanned by it, where $u = x \cap y, v = x \cup y$, let $X' = X \cap R(u, v)$. The segment $e = (x, y)$ is an edge of $conv(X)$ if and only if it is an edge of $conv(X')$.*

Proof. $\Rightarrow$: Necessity is oblivious. Suppose that $e = (x, y)$ is an edge of $conv(X)$, there exists a hyperplane $h(z) = 0$ which only supports vertices x and y in X. Since $X' \subseteq X$, $h(z) = 0$ is also the supporting hyperplane of $conv(X')$ on x and y, implying that $e = (x, y)$ is the edge of $conv(X')$.

$\Leftarrow$: To see sufficiency, suppose that $e = (x, y)$ is an edge of $conv(X')$. Denote $A = u \oplus v$. There exists a hyperplane $h_1(z) = w^\top z + b = 0$ such that

$$h_1(x) = h_1(y) = 0$$
$$\forall z \in X', z \neq x, z \neq y, h_1(z) > 0$$
$$\forall i \notin A, w_i = 0.$$

Therefore, for any $x \in X$, we have $h_1(z) = h(z \cap A)$. Hence, consider the hyperplane $h_2(z) = t^\top (z - u)$, where $t_i = C/(1 - 2u_i)$ for $i \notin A$. Then, for any z, we have $h_2(z) = t^\top (z - u) = C d_H(u, z \cap \overline{A})$, where d_H is the Hamming distance and $\overline{A}$ is the complement set of A.

Thus, for any $z \in R(u, v)$, we have $u = z \cap \overline{A}$ and $h_2(z) = 0$. For any $z \notin R(u, v)$, we have $d_H(u, \cap \overline{A}) \geq 1$, thus implying $h_2(z) \geq C$.

Let $h_3(z) = h_1(z) + h_2(z)$. For $z \in R(u, v)$, we have $h_3(z) = h_1(z)$. For $z \notin R(u, v)$, we have $h_3(z) \geq h_1(z) + C$. Since X is finite, there exist sufficient large constant C, such that $h_3(z) > 0$ for $z \notin R(u, v)$.

Combine the above, it is clear that $h_3(z) = 0$ supports X only on the point x and y, which means that $e = (x, y)$ is also an edge of $conv(X)$. $\square$

Generally, this lemma implies a strong locality. In other words, to determine whether a segment is an edge of the polytope, it suffices to only inspect the subcube spanned by the endpoints.

3.3 Polytope Graph

Definition 14. *For any polytope P, its polytope graph G is defined as $G = (V, E)$, where V is the set of extreme points of P and $(u, v) \in E$ if and only if it is an edge (1-face) of P.*

The polytope graph is an abstraction of the polytope by connecting the vertices with the edges of the polytope.

Specifically, for each edge $e \in E$, we define $w(e) = d_H(u, v)$, where $w(e)$ is the distance/weight of the edge e and $d_H(u, v) = |u \oplus v|$ is the Hamming distance.

Lemma 14. *Let G be the polytope graph of a 0/1 polytope P and $d_G(u, v)$ denote the length of shortest path between u and v in G, then we have $d_G(u, v) = d_H(u, v)$.*

PROOF. We prove this by induction.

Let $m = d_H(u, v)$. Take $m = 0$, we have $d_H(u, v) = 0 \implies u = v$, and the claim stands clearly.

Take $m = 1$, we have $d_H(u, v) = 1$. Notice that (u, v) is the edge of the hypercube. Therefore, (u, v) is also the edge of any 0/1 polytope that includes vertices u and v, $(u, v) \in E$ and $d_G(u, v) = w(e) = d_H(u, v)$. The claim also stands.

Suppose that the claim stands for any $m \in [0, k]$. Take $m = k + 1$. For any (u, v) with $d_H(u, v) = k + 1$, let $X' = R(u \cap v, u \cup v)$ and G' be the polytope graph of $conv(X')$. According to Lemma 13, G' is a subgraph of G, indicating that for any (u, v), $d_G(u, v) \leq d_{G'}(u, v)$.

Take any vertex t such that w is adjacent to u in G'. Since $t \in R(u \cap v, u \cup v)$, we have $d_H(u, t) + d_H(t, v) = d_H(u, v)$. Hence, by induction we have $d_{G'}(t, v) =$

$d_H(t, v)$ and $d_{G'}(u, t) = w(u, t) = d_H(u, t)$. Therefore, we have

$$\begin{aligned} d_G(u, v) &\leq d_G(u, t) + d_G(t, v) \\ &\leq d_{G'}(u, t) + d_{G'}(t, v) \\ &= d_H(u, t) + d_H(t, v) \\ &= d_H(u, v). \end{aligned}$$

Notice that by construction, we have $d_G(u, v) \geq d_H(u, v)$. Combine these to get $d_G(u, v) = d_H(u, v)$, thus completing the induction. □

Remark. Intuitively, this lemma implies that the shortest routing from u to v in the polytope graph G never takes a detour. Essentially, for any u, v, there exist $w_1, w_2, \cdots, w_k \in 2^{[n]}$, such that

$$\begin{gathered} u \subseteq w_1 \subseteq \cdots w_i \subseteq w_{i+1} \subseteq \cdots w_k \subseteq v, \\ (u, w_1), (w_k, v), (w_i, w_{i+1}) \in E(G), \forall i \in [k-1], \end{gathered}$$

and the chain $(u, w_1, \cdots, w_k, v)$ is a shortest path.

3.4 Computing USO Polytope

3.4.1 Computational Complexity

Though we properly define the USO polytope it is not feasible to compute all the faces of the USO polytope, even for P_3. Given a d-dimensional polytope P with r vertices, the problem to compute all the facets for P is referred to as facet-enumeration. Typical schemes to solve this includes randomized incremental construction[6], gift-wrapping method[25], and shelling method[23]. However, as we have $O(r^{\lfloor d/2 \rfloor})$ face in P_n, and $r \in n^{2^{\Theta(n)}}$ for USO polytope P_n by [18], it is not feasible to compute all the faces of P_n in practice.

Alternatively, we will investigate the 0, 1, and 2-faces of P_n instead, in which we do not enumerate all the faces and achieve affordable computational cost.

Remark. [28] shows that a general 0/1-polytope might have an exponential or super-exponential number of facets, while the number of faces in the USO polytope remains open. In the appendix, we provide some numerical estimations of the faces in P_3.

3.4.2 Vertex of USO polytope

Since P_n is a 0/1 polytope, each p_s is its vertex.

Proof. See Fact 11.

3.4.3 Edge of USO polytope

By 1, suppose that the segment (p_s, p_t) is a 1-face (edge), then there exists a hyperplane which only supports vertex p_s, p_t and excludes other vertices. To verify this, we check the feasibility of the following linear system.

$$w^\top p_u + b \geq 1, \forall u \notin \{s,t\},$$
$$w^\top p_s + b = w^\top p_t + b = 0.$$

If the above LP is feasible, (p_s, p_t) is an edge. Otherwise, it is not.

A straightforward way to understand the combinatorial meaning of the edge (p_s, p_t) is that flipping a set of edges L would transform the USO s into t, or vice versa. However, suppose that there are N different USOs, there are in total $\binom{N}{2}$ such flips. Not each such flip is an edge in P_n unless the USO Polytope is a simplex, which is not true.

Therefore, it raises the question that how can we distinguish edges and non-edges by their combinatorial meanings. Here we provide some sufficient conditions based on the phase decomposition.

Corollary 15. *Let P_n be the USO polytope of Q_n. Let s and t be different USOs and L is the set of edges whose orientations are different in s and t.*

Therefore, (p_s, p_t) is an edge of P_n if L is a single phase of s. Hence, (p_s, p_t) is not an edge if L is the union of multiple phases in s.

PROOF. Suppose L is a single phase of s, $L' \subsetneq L$, and another orientation s' is obtained by flipping all the edges among L' in s. According to Lemma 10, s' is not a USO. Therefore, p_s and p_t are the only two vertices in the subcube $R(p_s \cap p_t, p_s \cup p_t)$. By Lemma 13, the segment $e = (p_s, p_t)$ is an edge of the polytope P.

Besides, suppose that L is the union of multiple phases, $L = \bigcup_{i=1}^k l_i$, where $\forall i \in [k]$, l_i is a single phase of s and $k \geq 2$. Denote s_i as the orientation obtained by flipping the phase l_i in s, thus

$$p_t - p_s = \sum_{i=1}^{k} p_{s_i} - p_s$$

Let $X = \{s, t, s_1, s_2, \cdots, s_k\}$. Notice that $\forall i \in [k]$, s_i is also a USO, thus making p_{s_i} a vertex of P_n. By the above argument, we have (p_s, p_{s_i}) is the edge of P_n. Since $p_t - p_s$ is a conic combination of $p_{s_i} - p_s$, we have (p_s, p_t) is not an edge of $conv(X)$, thus not an edge of P_n. □

Algorithm 1 2-FACE DETECTION

Input: Polytope Graph $G_n = (V, E)$
Output: 2-Faces Set F.

1: $F \leftarrow \varnothing$
2: **for** $u \in V$ **do**
3:   **for** $(u, v) \in E, (u, w) \in E, v \neq w$ **do**
4:     $f \leftarrow \{u, v, w\}$
5:     **for** $p \in V$ **do**
6:       **if** $rank(p - u, v - u, w - u) = 2$ **then**
7:         $f \leftarrow f \cup \{p\}$
8:       **end if**
9:     **end for**
10:     **if** ISBOUNDARY(f) **then**
11:       $F \leftarrow F \cup \{f\}$
12:     **end if**
13:   **end for**
14: **end for**
15: **return** F

REMARK. Notice that in this lemma L is not required to be non-adjacent in s, which is a more general case than Lemma 10.

3.4.4 2-face of USO polytope

Let G_n be the polytope graph of P_n. Once we determine the edges of G_n, we can further aggregate the 2-faces of P_n by the following algorithm 2-FACE DETECTION.

Correctness. For each 2-face f, it can be represented by a 2-dimensional polygon $(p_1, p_2, \cdots, p_3)$, in which $(p_i, p_{i+1}) \in E$. In Lines 2-3, we iterate over all the possible 2-face by iterating over all the triplets (u, v, w) in which (u, v) and (u, w) are connected in G. Further, we find all the other vertex p such that $p - u \in span\{v - u, w - u\}$, which means p lies in this 2-dimensional subspace, aggregating into the 2-dimensional polygon f. Finally, ISBOUNDARY(f) verifies whether there exists a hyperplane that only supports the vertices set $V(f)$ and is implemented by checking the feasibility of the following linear system.

$$w^\top u + b \geq 1, \forall u \notin V(f),$$
$$w^\top u + b = 0, \forall u \in V(f).$$

Efficiency. Let $N = |V|, M = |E|, K = \sum_{u \in V} deg^2(u)$.

The nested loops in Lines 2-3 take in total $O(K)$ iterations. For each possible triplet (u, v, w), it takes $O(N)$ iterations to collect all the other vertices that lie in this spanned subspace. Further, it needs solving a linear program with $n2^{n-1} + 1$ variables and N constraints to check whether it exactly supports the polygon f. Since $n2^n \in o(N)$, the time complexity to solve this linear program is $O(N^\omega)$, where ω is the exponent of matrix multiplication with $\omega \approx 2.38$. Therefore, the overall runtime complexity is $O(N^\omega K + NK) = O(N^\omega K)$.

Acceleration. We accelerate the 2-Face Detection by efficiently computing all the possible 2-faces f, and such improvement is based on the following facts.

Fact 16. *Let P be a 0/1-polytope. For each 2-face f of P, f includes at most 4 vertices of P.*

Proof. We prove this by contradiction. Suppose there exists a 2-face f containing at least 5 vertices, $V(f) = (a, b, c, d, e)$. Denote $U = span\{b - a, c - a, d - a, e - a\}$, and we will show that $dim(U) \geq 3$.

W.L.O.G., we can suppose that $a = \mathbf{0}$. Otherwise, we could apply some linear transformation $T : \{0, 1\}^d \to \{0, 1\}^d$ to P_n such that $T(a) = \mathbf{0}$ and the $dim(U)$ remains unchanged. Thus, $U = span\{b, c, d, e\}$. Since b, c, d, e are distinct vertices and are not parallel to each other, $dim(U) \geq 2$. Suppose that $dim(U) = 2$ and $\{b, c\}$ is a basis of U.

Consider the following linear indeterminate equation.

$$bx + cy = t, t \in \{0, 1\}^d.$$

Since b and c are distinct, there exists i such that $b_i + c_i = 1$. Suppose that $b_i = 1$ and $c_i = 0$. Since $b_i x + c_i y \in \{0, 1\}$, we have $x \in \{0, 1\}$. Therefore, $(x, y) \in \{(0, 0), (0, 1), (1, 0)\}$ are valid solutions and $(x, y) = (1, 1)$ is valid if and only if $b + c \in \{0, 1\}^d$. Thus, at most 3 nonzero solutions can be achieved, leading to the contradiction. $\square$

This fact can be generalized to the following lemma.

Lemma 17. *Let P be a 0/1 polytope. For each k-face f of P, f includes at most 2^k vertices.*

Proof Sketch. This can be proved directly by applying induction on the above fact 16. $\square$

Fact 18. *Let P be a 0/1 polytope. For each 2-face f of P, if a 2-face f includes 4 vertices of P, f is a rectangle.*

Proof. According to Fact 14, if a 2-face f includes 4 vertices, it can be formulated as $V(f) = (t, t + a, t + b, t + a + b)$. Notice that $f \subseteq \{0, 1\}^d$, we have $\forall i, a_i b_i = 0$ and $a^\top b = 0$. Therefore, f is indeed a rectangle. □

Therefore, for each triplet (u, v, w), the only possible co-planar vertex other than (u, v, w) is $v + w - u$. Having utilized this, we could improve the efficiency of the 2-Face Detection.

Remark. Asymptotically, this acceleration does not improve the complexity. However, it helps us to get rid of $O(NK)$ times co-planar check, which is useful in practice.

3.5 Isometry

In this section, we will discuss the isomorphism between different USOs, and the isometry on the USO polytope itself. Intuitively, the structure of the USO polytope is highly symmetric. The isometry of the USO tells us about how to transform a USO s into another USO s' such that they are identical to each other, and the isometry of the USO polytope P_n talks about the symmetry group of P_n under which transformation P_n remains invariant.

An immediate benefit from the symmetry group is that it significantly improves the computation of the USO polytope. Suppose that we know a vertex u is identical to another vertex v in P_n, we only need to compute the local structure of u, which induces the information of v.

In the following context, we will properly define in which situation, USO s and s' can be regarded as identical to each other, and hence, the isometry group of the USO polytope.

3.5.1 Isomorphic USO

Definition 15. *Two USO s and s' on the hypercube Q^n are called isomorphic to each other if and only if there exists a mapping $f : V(Q_n) \to V(Q_n)$ such that $\forall (u, v) \in E(Q_n)$,*

$$(f(u), f(v)) \in E(Q_n),$$
$$I_s(u, v) = I_{s'}(f(u), f(v)).$$

Briefly, we can say (s, s') admits the isomorphism mapping f, and they are in the same isomorphism class, which means they are identical to each other.

Similarly, we say that s admit the automorphism mapping f if $\forall (u,v) \in E(Q_n)$,

$$(f(u), f(v)) \in E(Q_n),$$
$$I_s(u,v) = I_s(f(u), f(v)).$$

The isomorphism of USO is defined as equivalent to the isomorphism of the directed graph. For general graph G and G', it may have $|V(G)|!$ potential isomorphism f, which is a bijection from $V(G)$ to $V(G')$. However, as Q_n is a highly symmetric regular graph, we can see that the size of the isomorphism mapping is much smaller than $|V(Q_n)|!$, and can be easily described as the composition of basic mappings.

For this purpose, first, we introduce some basic mappings.

Definition 16. *Let f mapping on $2^{[n]}$, $f : 2^{[n]} \to 2^{[n]}$.*
An identical mapping f is that $f(u) = u$.
A reflection f characterized by $r \in \{0,1\}^n$ is that $f(u) = u \oplus r$.
A rotation f characterized by $\sigma \in \mathbf{S_n}$ is that $f(u)_{\sigma(i)} = u_i$, where $\mathbf{S_n}$ is the group of all the permutations on $[n]$.

In a nutshell, a reflection reflects the hypercube with regard to certain directions and a rotation permutes a certain axis of the hypercube around $\varnothing$.

To characterize the isomorphism of the hypercube, we need some other auxiliary lemmas at first.

Lemma 19. *Given a fixed vertex $u \in Q_n$ and let $N(u)$ be the set of its neighbors in Q_n, for any vertex $v \in Q_n$, it can be uniquely characterized by the distance between v and $u \cup N(u)$.*

In other words, denote $T(u) = u \cup N(u) = \{u_1, u_2, \cdots, u_{n+1}\}$, the function $\Gamma : \{0,1\}^n \to [0,n]^{n+1}$ is injective, where

$$\Gamma(v)_i = d_H(v, u_i), \forall i \in [n+1].$$

Proof. W.L.O.G., suppose $u = \mathbf{0}$. Notice that for any $w \in N(u)$, we have

$$|d_H(u,v) - d_H(w,v)| = 1.$$

Suppose $w_\lambda = 1$. If $d_H(u,v) < d_H(w,v)$, we have $v_\lambda = u_\lambda = 0$. Otherwise, we have $v_\lambda = w_\lambda = 1$. Therefore, for any $\lambda \in [n]$, v_λ is determined its distance from u and $w = \{\lambda\}$, thus making Γ injective. $\square$

Corollary 20. *For any automorphism mapping f of the hypercube Q_n and a fixed vertex $u \in Q_n$, f is uniquely determined by the mapping of u and its neighbor set $N(u)$.*

Proof. Notice that for any (u, v), we have $d_H(u, v) = d_H(f(u), f(v))$. According to Lemma 19, v is uniquely determined by $\Gamma(v)$. Since $\Gamma(v) = \Gamma(f(v))$, $f(v)$ is also uniquely determined. Hence, the automorphism mapping f itself is unique as well. □

We can see that the mapping of $T(u) = u \cup N(u)$ is a basis of f, and it determines f immediately. Hence, we will further argue that the mapping of u and $N(u)$ can be regarded as a composition of reflection and rotation.

Lemma 21. *For any isomorphism mapping f between USOs s and s', it must be composed of a rotation g and a reflection h such that $f = g \circ h$.*

Proof. Since f is isomorphism mapping between s and s', it is also an automorphism mapping of the hypercube Q_n. It suffices to argue the case for the hypercube: if the hypercube Q_n admits an automorphism f, f can be decomposed as $f = g \circ h$.

According to 20, suppose that $f(z) = \mathbf{0}$, then f can be decomposed into a reflection $h(u) = u \oplus z$ which is mapping u to $\mathbf{0}$ and a rotation g which is mapping $N(u)$ to $N(\mathbf{0})$. Hence, for any such bijective mapping $g : u \cup N(u) \to \mathbf{0} \cup N(\mathbf{0})$, the automorphism f that agrees with g is unique. □

Remark. As is a direct implication from Lemma 21, we can see that there are $2^n n!$ types of automorphism on the hypercube Q_n: We have 2^n types of reflection and $n!$ types of rotation, and different combinations of them induce different automorphism because we either map different u to $\mathbf{0}$ or map the neighbors of u differently.

3.5.2 Isomorphism Classes

Denote the set of all USOs of Q_n as U_n and the group of all possible isomorphism mapping on Q_n as F_n respectively. For $s, s' \in U_n$, they are in the same isomorphism class under F_n if there exists $f \in F_n$ such that $f(s) = s'$. Denote U_n/F_n as the set of isomorphism classes of U under F_n. According to Burnside's Lemma [5],

$$|U_n/F_n| = \frac{1}{|F_n|} \sum_{f \in F_n} \phi(f),$$

where $\phi(f) = |\{s | f(s) = s, s \in U_n\}|$, which is the number of fixed points under isomorphism mapping f.

By [18], we can see that $|U_n/F_n|$ is asymptotically same as $|U_n|$, as $|U_n/F_n| \geq |U_n|/|F_n|$, and $|F_n| = 2^n n!$ is negligible compared to $|U_n|$. However, it could still better our understanding of the structure of isomorphism classes if we could estimate the number of fixed points of a specific hypercube automorphism f.

In the following lemma, we provide a sufficient condition for f such that it has nonzero fixed points.

Definition 17. *Let $\sigma \in S_n$, the cyclic decomposition C of σ is defined as*

$$C = \{c_1, c_2, \cdots, c_m\},$$
$$\forall i \in [m], c_i = (x_{i,1}, x_{i,2}, \cdots, x_{i,k_i}),$$
$$\forall i \in [m], j \in [k_i], \sigma(x_{i,j}) = x_{i,(j \mod k_i)+1},$$
$$\forall i \in [m], j \in [m], i \neq j, c_i \cap c_j = \varnothing.$$

Lemma 22. *Let F_n be the group of all possible isomorphism mapping on Q_n. For any $f \in F_n$ and its decomposition $f = g \circ h$, $h(u) = u \oplus r$ is a reflection and $g(u)_{\sigma(i)} = u_i$ is a rotation, where $\sigma \in \mathbf{S_n}$.*

Let C be the cyclic decomposition of σ and $\forall c_i \in C$ let $\kappa(c_i) = \{k | k \in c_i\}$ and $\tau = \{k | r_k = 1\}$.

Then, if for any $c_i \in C$, $|\kappa(c_i) \cap \tau|$ is even, $\phi(f) \neq 0$.

PROOF. Generally, we prove this by finding a uniform USO that admits such f.

In a uniform USO s, for any λ-edge e, we have

$$I_s(e) = I_{s,\lambda}, \lambda \in [n],$$

and the uniform USO s can be characterized by the indicator $I_s = (I_{s,1}, I_{s,2}, \cdots, I_{s,n})$. Denote s' as the orientation obtained by operating transformation f on s.

Apart from the reflection h, let us only consider the permutation $g(u)_{\sigma(i)} = u_i$ at first. For any λ-edge (u, v), we have

$$u \oplus v = \lambda,$$
$$g(u) \oplus g(v) = \sigma(\lambda),$$

which shows that g is mapping each λ-edge in s to a $\sigma(\lambda)$-edge in s' and we have $I_{s,\lambda} = I_{s',\sigma(\lambda)}$.

Next, we take the reflection h into consideration. For any λ-edge (u, v) with $u \oplus v = \lambda$, we have

$$g(h(u))) \oplus g(h(v)) = g(u) \oplus g(r) \oplus g(v) \oplus g(r) = \sigma(\lambda),$$

where $f = g \circ h$ is also mapping λ-edges in s to a $\sigma(\lambda)$-edges in s'.

Hence, let $u \subseteq v$, $f(u) \subseteq f(v)$ if and only if $\lambda \notin r$. Therefore,

$$I_{s',\sigma(\lambda)} = \begin{cases} I_{s,\lambda}, & \lambda \notin r, \\ 1 - I_{s,\lambda}, & \lambda \in r. \end{cases}$$

Assuming that s admits the automorphism f, we have $I_s = I_{s'}$.

Hence, since each cycle c_i is disjoint we can consider them independently since they are operated on edges of different directions. Therefore, we can assume that $C = \{c_1\}$ and $|c_1| = n$. It is clear that as long as $|r|$ is even, the above linear system has a feasible solution. □

3.5.3 Isomorphic Polytope

Motivation A good example to see why we need to seek the isometry of USO polytope for its combinatorial meanings is as follows:

Notice that for any USO s, and the USO s' obtained by flipping all its edges, we have

$$I_s(e) + I_{s'}(e) = \mathbf{1},$$
$$p_s + p_{s'} = \mathbf{1},$$

which indicates that the USO polytope is central symmetric around the point $p_c = (1/2, 1/2, \cdots, 1/2)$.

Next, let us fix the s and s' to be specific ones. Let s be a uniform USO of Q_n with $n \geq 3$, u be its unique sink and $e = (u, v)$ be an edge incident to u. Let s_1 be the USO obtained by flipping e in s, and s_2 be the USO obtained by flipping all the edges in s_1. Thus, we have $p_{s_1} + p_{s_2} = \mathbf{1}$, and the USO polytope should look the same in the points of view at p_{s_1} and p_{s_2}.

However, s_1 and s_2 are not isomorphic to each other because s_1 differs from a uniform USO by an edge incident to the unique sink but s_2 differs by an edge incident to the unique source, which means that although two vertices of the USO polytope are considered geometrically equivalent, of which the notion will be defined later, their associated USO does not necessarily be isomorphic.

To discuss the geometry isometry of the USO polytope, we need to first properly define the isometry.

Definition 18. *An isometry in the Euclidean space R^d is a transformation $f : R^d \to R^d$ such that $\forall x, y$, $\|x - y\|_2 = \|f(x) - f(y)\|_2$, and the group of such isometry is denoted as* $\mathbf{SE_d}$.

The image of P under the isometry f is denoted as $f(P)$, and

$$f(P) = \{f(x)|x \in P\}.$$

For any d-dimensional polytope P and Q, P is isomorphic to Q is there exists $f \in \mathbf{SE_d}$ such that $Q = f(P)$ and $P = f^{-1}(Q)$. Specifically, we say that P admits an automorphism f on itself if $P = f(P)$.

Similar to the isomorphism of the hypercube, the isometry in $\mathbf{SE_d}$ is also composed of the basic isometry.

Definition 19. *A d-dimensional Euclidean isometry f is called*

- *translation, if $f(u) = u + c, c \in R^d$.*
- *rotation, if $f(u) = Au$, where A is an orthogonal matrix in $R^{d\times d}$.*
- *reflection, if $f(u) = u - 2\frac{w^\top u+b}{w^\top w}w$, where $H = w^\top x + b = 0$ is the hyperplane that characterizes this reflection.*

Lemma 23. $\mathbf{SE_d}$ *is composed of any finite composition of translations, rotations, and reflections in R^d.*

Proof. See chapter 1.2 rigid transformation in [8].

Theorem 24. *Let P and Q be d-dimensional polytopes and $X = V(P), Y = V(Q)$ be the vertex sets of them respectively. Then, for any $f \in \mathbf{SE_d}$, $f(P) = Q$ if and only if $f(X) = Y$.*

Proof. $\Rightarrow$: Suppose that $f(P) = Q$. We argue that $x \in X \Leftrightarrow f(x) \in Y$.

Suppose $x \in X$, there exists a supporting hyperplane H of P such that $H \cap P = \{x\}$. By Lemma 23, $f(H)$ is the supporting hyperplane of $f(P)$ and $f(H) \cap f(P) = \{f(x)\}$, thus making $f(x)$ a vertex of the image Q and $f(x) \in Y$.

Vice versa, suppose $f(x) \in Y$, the similar argument stands, as $f^{-1} \in \mathbf{SE_d}$ and we have $X = f^{-1}(Y), x = f^{-1}(f(x)) \in X$, and this concludes the proof of the sufficiency.

$\Leftarrow$: Suppose that $f(X) = Y$. We need to argue that $x \in P \Leftrightarrow f(x) \in Q$.

By Lemma 23, it is clear that for $f \in \mathbf{SE_d}, f(x) = y$, each coordinate y_i is a nonhomogeneous linear combination of x_i, such that

$$y_i = B_i + \sum_{j=1}^{d} A_{i,j} x_j,$$

where $A \in R^{d\times d}, B \in R^d$. Accordingly, we can extend f to another isometry g which is embedded on a hyperplane of R^{d+1} such that $\forall x \in R^d$,

$$h(x) = \begin{bmatrix} x \\ 1 \end{bmatrix},$$

$$g(h(x)) = \begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} = \begin{bmatrix} f(x) \\ 1 \end{bmatrix} = h(f(x)).$$

In other words, g is homogeneous linear transformation characterized by the matrix $\Gamma = \begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}$, such that $g(x) = \Gamma x$. Meanwhile, denote $M(P) \in R^{d\times n}$ as the matrix whose columns are $V(P)$.

Suppose that $x \in P$, it is a convex combination of X, which means that there exist $\Lambda = (\lambda_1, \lambda_2, \cdots, \lambda_n)$, $\lambda_i \geq 0$ and $\sum_{i=1}^{n} \lambda_i = 1$, such that $x = M(P)\Lambda$. Therefore,

$$g(h(x)) = \underbrace{\begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} X_1 & \cdots & X_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(P))} \underbrace{\begin{bmatrix} \lambda_1 \\ \cdots \\ \lambda_n \end{bmatrix}}_{\Lambda} = h(f(x)).$$

Since $f(X) = Y$, we have

$$\underbrace{\begin{bmatrix} A & B \\ 0 & 1 \end{bmatrix}}_{\Gamma} \underbrace{\begin{bmatrix} X_1 & \cdots & X_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(P))} = \underbrace{\begin{bmatrix} Y_1 & \cdots & Y_n \\ 1 & \cdots & 1 \end{bmatrix}}_{h(M(Q))},$$

$$f(X_i) = Y_i.$$

Therefore, $g(h(x)) = h(M(Q))\Lambda$. For any $x \in P$, $g(h(x)) = h(f(x))$ is also a convex combination of $h(M(Q))$, indicating $h(f(x)) \in h(Q)$, thus $f(x) \in Q$.

Vice versa, suppose $f(x) \in Q$, the similar argument also stands. Take $f^{-1} \in \mathbf{SE_d}$ and $P = f^{-1}(Q), x = f^{-1}(f(x)) \in P$, thus proving the necessity. $\square$

This theorem shows that instead of considering the compact polytope, it is enough to only focus on the bijection between vertices of the polytope. Nevertheless, the number of such bijections grows exponentially with regard to the number of vertices in P. Therefore, we need further refine the scope of the isometry on the USO polytope.

For further analysis, two basic but important facts are needed.

Fact 25. *Let P_n be the USO polytope of Q_n and s be a uniform USO. Let t_i be the USO obtained by flipping the i-th edge in s. Let G be the polytope graph of P_n and $N(u)$ be the set of neighbors of u in G. Then, we have*

$$N(p_s) = \{p_{t_i} | i \in [m], m = n2^{n-1}\}.$$

PROOF. First, we need to argue that each t_i is indeed a USO. Notice that for a uniform USO s and its outmap S, we have

$$S(u) = u \oplus z,$$

where z is the unique sink of s in Q_n. Therefore, for two λ-edges e_1, e_2 and $u \in e_1, v \in e_2$, we have

$$(u \oplus v) \cap (S(u) \oplus S(v)) = (u \oplus v) \cap (u \oplus z \oplus v \oplus z) = u \oplus v.$$

Notice that $u \oplus v = \{\lambda\}$ only if u, v belong to the same λ-edge. Thus, for any two λ-edges e_1, e_2, they are not in direct phase to each other. For any edge e_i in s, the phase of it is $\{e_i\}$, which means only flipping itself will lead to another USO t_i.

Next we argue that $N(p_s) = \{p_{t_i | i \in [n2^{n-1}]}\}$. For any USO t other than s, denote L as the set of edges that have different orientations in s and t. Notice that s is a uniform USO and no two edges are in the same phase. Therefore, L is always a union of single or multiple phases. By corollary 15, (p_s, p_t) is the edge of P_n if and only if $|L| = 1$, indicating that $N(p_s) = \{p_{t_i} | i \in [m], m = n2^{n-1}\}$. $\square$

REMARK. Notice that $U = \{p_{t_i} - p_s | i \in [m]\}$ is an orthogonal basis of the space R^m, we have $dim(P_n) = n2^{n-1}$, which implies that P_n is full ranked.

Corollary 26. *Let P_n be the USO polytope of Q_n and s be a uniform USO. Let G be the polytope graph of P_n and $N(u)$ be the set of neighbors of u in G.*

Suppose that P_n admit an automorphism $f \in \mathbf{SE_m}, m = n2^{n-1}$, then for any USO t of Q_n, $f(p_t)$ can be uniquely determined by the $f(p_s)$ and $f(N(p_s))$.

PROOF. For simplicity, we write $t_0 = s$ and let t_i be the orientation which differs from t_0 by the orientation of the i-th edge.

Let $U = \left[p_{t_0} \dots p_{t_m}\right]$. Hence, notice that $\{p_{t_i} - p_{t_0} | i \in [m]\}$ is an orthogonal basis of the space $\{0,1\}^m$ and $p_{t_i} \in \{0,1\}^m$. Therefore, for any $y \in \{0,1\}^m$, y belongs to the affine hull of the columns of U, and there exists $\lambda \in R^{m+1}$ with $\sum_{i=0}^m \lambda_i = 1$ such that $y = U\lambda$.

by Lemma 23, $\forall f \in \mathbf{SE_m}$, we have $f(x) = w^\top x + b$, where $w, b \in R^m$. Therefore,

$$
\begin{aligned}
f(y) &= w^\top U\lambda + b \\
&= b + \sum_{i=0}^{m} \lambda_i w^\top p_{t_i} \\
&= b + \sum_{i=0}^{m} \lambda_i (f(p_{t_i}) - b) \\
&= \sum_{i=0}^{m} \lambda_i f(p_{t_i}),
\end{aligned}
$$

indicating that $f(p_t)$ is characterized by the mapping of p_s and its neighbours $N(p_s)$. $\square$

Remark. This proof is almost the same as the proof of corollary 26.

Recall that in theorem 24, we prove that the automorphism of the USO polytope is indeed a bijection of the vertices. Hence, notice that for each hypercube isomorphism f, it always transforms a USO s into another USO s', which is a bijection on the USOs. Therefore, it is straightforward to conjecture that such bijection always corresponds to an automorphism k of the USO polytope and $k \in SE_m$, which is proved in the next fact.

Fact 27. *Let F_n be the group of isomorphism on the hypercube Q_n and K_n be the group of automorphism on the USO polytope P_n, where $K_n \subseteq \mathbf{SE_m}, m = n2^{n-1}$.*

Then, for each $f \in F_n$, it induces a unique automorphism k such that for each USO s and s' with $f(s) = s'$, we have $k(p_s) = p_{s'}$.

Proof. Indeed, we only need to explicitly construct k such that $k \in \mathbf{SE_m}$. Let k be the automorphism in K_n induced by f, and $idx(e)$ be the index of the edge e fixed by the total order in section 3.1. By lemma 23 and corollary 26, $k = g \circ h$, where g is a rotation and h is a reflection.

For $e_1 = (u_1, v_1), e_2 = (u_2, v_2) \in E(Q_n)$, we denote $f(e_1) = e_2$ if $f(\{u_1, v_1\}) =$

$\{u_2, v_2\}$. Respectively, we construct g and h as follows. For $f(e_1) = e_2$, let

$$\sigma(idx(e_1)) = idx(e_2),$$
$$g(u)_{\sigma(i)} = i.$$

Hence, for any $f(e_1) = e_2$, let

$$[idx(e_1) \in r] = \begin{cases} 0, & f(u_1) \subseteq f(v_1), \\ 1, & f(v_1) \subseteq f(u_1). \end{cases}$$
$$h(u) = u \oplus r.$$

Therefore, for USOs s and s' with $f(s) = s'$, it is clear that $k(p_s) = p_{s'}$. □

By fact 27, we can see that $|F_n| \leq |K_n|$. However, by the examples we see in the **Motivation**, it is also clear that $|F_n| < |K_n|$, and there exists $k \in K_n$ such that k is not induced by any f. It is interesting to investigate the number and structure of k, and we address this by the following beautiful theorem 29.

Intuitively speaking, for any $k \in K_n$, let f be the mapping of USO such that for any USO s and s' with $k(p_s) = p_{s'}$, we have $f(s) = s'$. Indeed, f is transforming s into s', but not always in an isomorphic way. We will show that f is composed of a hypercube isomorphism and flipping some edges in certain directions.

To prove this, we need the following lemma about the bijection of hypercube edges at first.

Lemma 28. *Let f be bijection on $E(Q_n)$ such that $\forall e_1, e_2, f(e_1), f(e_2)$ are adjacent if and only if e_1, e_2 are adjacent.*

Then, f is actually induced by some $g \in F_n$ such that $\forall \{u, v\} \in E(Q_n)$, we have $f(\{u, v\}) = \{g(u), g(v)\}$.

Proof. Construct g explicitly. For each vertex $u \in V(Q_n)$, consider all the edges $e_1, e_2, \cdots, e_n$ incident to the vertex u, we have

$$e_1 \cap e_2 \cap \cdots \cap e_n = \{u\}.$$

Notice that $f(e_i)$ are also adjacent to each other pairwise and Q_n is a regular graph of degree n. Therefore, there exists v such that

$$f(e_1) \cap f(e_2) \cap \cdots \cap f(e_n) = \{v\},$$

and let $g(u) = v$ in this case. It is clear that g is uniquely determined by f and for each $g \in F_n$, the induced f also preserves the adjacency of the edges. □

Next, we conclude the section with the following theorem.

Theorem 29. *Let K_n be the group of automorphism of USO polytope P_n.*

Then, $\forall k \in \mathbf{SE_m}, m = n2^{n-1}$, $k \in K_n$ ***if and only if*** *$k = g \circ h$, where h is a reflection induced by $A \subseteq [n]$ and g is a bijection on $[m]$ induced by some $f \in F_n$.*

PROOF. "$\Rightarrow$": Let k be a USO polytope automorphism and let $k(p_s) = \mathbf{0}$. It is obvious that s is a uniform USO, then k can be characterized on the reflection $h(u) = u \oplus p_s$ and the bijection g on the neighbors of p_s, and $k = g \circ h$.

By fact 25, we see that the bijection of the neighbors of s is indeed a bijection of $E(Q_n)$.

Hence, for any uniform USO s, denote $s(L)$ as the orientation obtained by flipping edges in L from s. Therefore, $\forall e \in E(Q_n)$, we have $s(\{e\})$ is another USO, and $\forall e_1, e_2 \in E(Q_n)$, $s(\{e_1, e_2\})$ is another USO if and only if e_1 and e_2 are not adjacent.

Let g further be an bijection of $E(Q_n)$, and $t = s(\{e_1, e_2\})$, then

$$k(p_s) = p_{s'},$$
$$k(p_t) = p_{s'(\{g(e_1), g(e_2)\})},$$

where s' is another uniform orientation. Therefore, $g(e_1)$ and $g(e_2)$ are adjacent if and only if e_1 and e_2 are adjacent.

By lemma 28, g is induced by some $f \in F_n$, which completes the proof of the necessity.

"$\Leftarrow$": To see sufficiency, by fact 27, for each $f \in F_n$, there exists a $j \in K_n$ induced by it, where $j = g \circ r$, where g is a permutation of edges and r is the reflection on certain direction $A \subseteq [n]$.

Compose j with any h' which represents flipping edges in certain directions A, then $k = j \circ h' = g \circ r \circ h = g \circ h$. By Lemma 2, flipping all the edges in some directions provides us with another USO. Therefore,

$$\forall p_s \in P_n, k(p_s) \in P_n.$$

Hence, k is bijective, indicating that $k \in K_n$. □

REMARK. As a direct result of theorem 27, we have $|F_n| = n!2^n, |K_n| \leq n!2^{2n}$.

4 Open Questions

We conclude with several open conjectures and potential further discussions, and some are based on some interesting observations in our practice.

- For USOs s and s' which differs in edge set L, one may conjecture that L always contains a complete phase l_i in s. However, it is not the case but there is only one counter-example for $n = 3$. What is the case for higher dimensions?
- Lemma 7 provides a necessary condition for the USO outmap. If we augment the condition by requiring each subcube to have such property, what combinatorial structure will we get?
- Corollary 15 conclude the case where edges being flipped can be decomposed into phases, what about the case where edges are intersecting but not a union of phases?
- Lemma 22 provides a sufficient condition for an automorphism to have non-zero fixed points. However, in practice, it is also the necessary condition for $n = 3$. What is the case in a higher dimension?
- Lemma 29 show that $|K_n| \leq 2^{2n}n!$. It is further conjectured that $|K_n| = 2^{2n}n!$, which means the different composition of flips and hypercube isomorphism would induce different USO polytope automorphism.

References

[1] Garrett Birkhoff. Three observations on linear algebra. *Univ. Nac. Tacuman, Rev. Ser. A*, 5:147–151, 1946.

[2] Karol Borsuk. Drei sätze über die n-dimensionale euklidische sphäre. *Fundamenta Mathematicae*, 20(1):177–190, 1933.

[3] Michaela Borzechowski, Joseph Doolittle, and Simon Weber. A universal construction for unique sink orientations. *arXiv preprint arXiv:2211.06072*, 2022.

[4] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, March 2004.

[5] William Burnside. *On the isomorphism of a group with itself*. Cambridge Library Collection - Mathematics. Cambridge University Press, 2012.

[6] Bernard Chazelle. An optimal convex hull algorithm in any fixed dimension. *Discrete & Computational Geometry*, 10(4):377–409, 1993.

[7] Jan Foniok, Bernd Gärtner, Lorenz Klaus, and Markus Sprecher. Counting unique-sink orientations. *Discrete Applied Mathematics*, 163:155–164, 2014.

[8] A.I.R. Galarza and J. Seade. *Introduction to Classical Geometries*. Birkhäuser Basel, 2007.

[9] Yuan Gao, Bernd Gärtner, and Jourdain Lamperski. A new combinatorial property of geometric unique sink orientations. *arXiv preprint arXiv:2008.08992*, 2020.

[10] Bernd Gärtner. The random-facet simplex algorithm on combinatorial cubes. *Random Structures & Algorithms*, 20(3):353–381, 2002.

[11] Bernd Gärtner, Walter D Jr. Morris, and Leo Rüst. Unique sink orientations of grids. *Algorithmica*, 51(2):200–235, 2008.

[12] Bernd Gärtner and Ingo Schurr. Linear programming and unique sink orientations. In *Proceedings of the Seventeenth Annual ACM-SIAM Symposium on Discrete Algorithm*, SODA '06, page 749–757, USA, 2006. Society for Industrial and Applied Mathematics.

[13] Hugo Hadwiger, Hans Debrunner, and Victor Klee. *Combinatorial geometry in the plane*. Courier Corporation, 2015.

[14] Martin Jaggi. *Linear and Quadratic Programming by Unique Sink Orientations*. PhD thesis, Diploma thesis, Institute for Theoretical Computer Science, ETH Zurich, 2006.

[15] Jeff Kahn and Gil Kalai. A counterexample to borsuk's conjecture. *Bulletin of the American Mathematical Society*, 29(1):60–62, 1993.

[16] Lorenz Klaus. On classes of unique-sink orientations arising from pivoting in linear complementarity. Master's thesis, ETH, Eidgenössische Technische Hochschule Zürich, Institute for Operations . . . , 2009.

[17] John Mackey. A cube tiling of dimension eight with no facesharing. *Discrete & Computational Geometry*, 28:275–279, 2002.

[18] Jiří Matoušek. The number of unique-sink orientations of the hypercube. *Combinatorica*, 26(1):91–99, 2006.

[19] Peter McMullen. The maximum numbers of faces of a convex polytope. *Mathematika*, 17(2):179–184, 1970.

[20] Eberhard Melchior. Uber vielseite der projektiven ebene. *Deutsche Math*, 5(1):461–475, 1940.

[21] Ingo Schurr and Tibor Szabó. Finding the sink takes some time: An almost quadratic lower bound for finding the sink of unique sink oriented cubes. *Discrete & Computational Geometry*, 31(4):627–642, 2004.

[22] Ingo A Schurr. *Unique sink orientations of cubes*. PhD thesis, ETH Zurich, 2004.

[23] Raimund Seidel. Constructing higher-dimensional convex hulls at logarithmic cost per face. In *Proceedings of the eighteenth annual ACM symposium on Theory of computing*, pages 404–413, 1986.

[24] Alan Stickney and Layne Watson. Digraph models of bard-type algorithms for the linear complementarity problem. *Mathematics of Operations Research*, 3(4):322–333, 1978.

[25] Garret Swart. Finding the convex hull facet by facet. *Journal of Algorithms*, 6(1):17–48, 1985.

[26] James Joseph Sylvester. Mathematical question 11851. *Educational Times*, 59(98):256, 1893.

[27] T. Szabo and E. Welzl. Unique sink orientations of cubes. In *Proceedings 42nd IEEE Symposium on Foundations of Computer Science*, pages 547–555, 2001.

[28] Günter M Ziegler. Lectures on 0/1-polytopes. In *Polytopes—combinatorics and computation*, pages 1–41. Springer, 2000.

A Faces in P_3

Dimension	0-Faces	1-Faces	2-Faces	Triangular 2-Faces	Rectangular 2-Faces
Number	744	30364	314122	291658	22464

The above table provides us with the numbers of low dimensional faces in P_3 acquired by algorithm 1.

B Isomorphism Class of U_3

Size	8	24	48	48	48	48	24	48	24	24
Degree	12	24	24	18	87	87	101	72	84	24
Size	48	48	48	48	48	48	48	48	16	
Degree	72	72	87	139	72	163	87	170	170	

There are in total 19 different isomorphism classes in U_3. The above table shows their sizes and degrees in the polytope graph G_3. Notice that different isomorphism classes may share the same degree as they might be geometrically equivalent.

C Fixed Points of F_3

σ \ r	$\varnothing$	$\{1\}$	$\{2\}$	$\{1,2\}$	$\{3\}$	$\{1,3\}$	$\{2,3\}$	$\{1,2,3\}$
$(1,2,3)$	744	0	0	0	0	0	0	0
$(1,3,2)$	20	0	0	0	0	0	20	0
$(2,1,3)$	20	0	0	20	0	0	0	0
$(2,3,1)$	6	0	0	6	0	6	6	0
$(3,1,2)$	6	0	0	6	0	6	6	0
$(3,2,1)$	20	0	0	0	0	20	0	0

For any hypercube isomorphism $f \in F_n$, it can be decomposed as $f = g \circ h$, where $g(u) = u \oplus r$ and $h(u)_{\sigma(i)} = u_i$. Notice that the decomposition is converse to the definition in 21, but it also defines the same isomorphism group F_n. The above table shows the number of fixed points in each $f \in F_n$.